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Bounding the Lebesgue Function for Lagrange Interpolation in a Simplex

L. P. Bos*

Department of Mathematics, University of Toronto, Toronto, Canada M5S 1A1

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1. Introduction

Denote the space of polynomials of degree n in m variables by $\mathbb{P}_n^m$ and let $X \subset \mathbb{R}^m$ be compact. It is well known that $\dim \mathbb{P}_n^m = \binom{n+m}{m} =: N_n^m$ (N when there is no ambiguity present; see, e.g., [2, p. 98]). Hence N_n^m conditions are needed to determine a polynomial uniquely.

The interpolation problem is then: given N_n^m distinct points, $x_i \in X$, and a function $f \in \mathscr{C}(X)$, find that $p \in \mathbb{P}_n^m$ satisfying $p(x_i) = f(x_i)$, $1 \leqslant i \leqslant N$. If we let $\{m_i(x)\colon 1 \leqslant i \leqslant N\}$ be a basis for $\mathbb{P}_n^m$, then this is equivalent to finding N_n^m numbers, $a_j \in \mathbb{R}$, so that

$$\sum_{j=1}^{N} a_j m_j(x_i) = f(x_i), \qquad 1 \leqslant i \leqslant N;$$

a linear system solvable for all right-hand sides iff its determinant is nonzero. We will refer to this determinant again and give it a name, $\mathrm{VDM}(x_1, x_2, ..., x_N)$, in recognition of the fact that in one dimension, if the basis is chosen to be $m_i(x) = x^{i-1}$, it is but the Vandermonde determinant.

An equivalent geometrical condition for all such interpolating polynomials to exist is that the points do not lie on the zero set of any nontrivial $q \in \mathbb{P}_n^m$.

Now consider a configuration of points with $\mathrm{VDM}(x_1, x_2, ..., x_N) \neq 0$. A very useful thing to do is to form the associated Lagrange polynomials l_i of degree n defined by the conditions $l_i(x_j) = \delta_{ij}$, $1 \leqslant i, j \leqslant N$. Then for $f \in \mathscr{C}(X)$, $(\prod_n f)(x) := \sum_{i=1}^{N} f(x_i)\, l_i(x)$ is its interpolating polynomial. By the uniqueness of solutions of nonsingular linear systems, $\prod_n(p) = p$ for all $p \in \mathbb{P}_n^m$ and hence the mapping $\prod_n\colon \mathscr{C}(X) \to \mathbb{P}_n^m$ is a projection.

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When both spaces are equipped with the supremum norm, the norm of this projection is well known and is easily seen to be

$$\left\|\prod_n\right\| = \max_x \sum_{i=1}^{N} |l_i(x)|.$$

The function $\Lambda(x) = \sum_i |l_i(x)|$ is usually referred to as the Lebesgue function of the interpolation process.

This norm is of interest for the following two reasons:

(i) If P_n^* is the best uniform approximation to f on X, then

$$\left\|f - \prod_n f\right\| \leqslant \left(1 + \left\|\prod_n\right\|\right) \|f - P_n^*\|.$$

Thus $\|\prod_n\|$ yields an estimate on how close the interpolation is to f.

(ii) For $p \in \mathbb{P}_n^m$,

$$\|p\| \leqslant \left\|\prod_n\right\| \max_{1 \leqslant i \leqslant N} |p(x_i)|.$$

Thus $\|\prod_n\|$ yields a simple method of bounding polynomials.

It is now clear that problems of interest are to first of all bound $\|\prod_n\|$ for a given set of points and secondly to find points for which this norm is small, if not as small as possible. Kilgore [4] and deBoor and Pinkus [1] have recently proven conjectures of Bernstein and Erdös characterizing these best points for the case of an interval $m = 1$. It is the purpose of this paper to discuss the case $m > 1$ and $X = T_m$, an m-dimensional simplex. We first show that the Lebesgue function for the "equally spaced" points is bounded by $\binom{2n-1}{n}$ independent of the dimension. Points with smaller norms are sought for by considering those which maximize |VDM|. They are calculated for low degrees and bounds for the Lebesgue function given.

2. Equally Spaced Points on a Simplex

It is convenient to use barycentric coordinates. Let v_i, $1 \leqslant i \leqslant m + 1$, be the vertices of T_m. Then any $x \in T_m$ can be written as a convex combination of the vertices:

$$x = \sum_{i=1}^{m+1} \lambda_i v_i, \qquad \sum_{i=1}^{m+1} \lambda_i = 1, \quad \lambda_i \geqslant 0.$$

The "equally spaced" points of degree n are then those points whose barycentric coordinates are of the form

$$(k_1/n, k_2/n, \ldots, k_{m+1}/n), \qquad k_i \text{ nonnegative integers.}$$

A little combinatorics shows that the number of such points is exactly N_n^m.

Now, simple formulas for the Lagrange polynomials are readily available. In fact, if we label the points $x_{\mathbf{k}} = (k_1/n, \ldots, k_{m+1}/n)$, where $\mathbf{k} = (k_1, k_2, \ldots, k_{m+1})$, then

$$l_{\mathbf{k}} = \left(n^n \Big/ \prod_{i=1}^{m+1} k_i!\right) \prod_{i=1}^{m+1} \prod_{k=0}^{k_i-1} (\lambda_i - k/n). \tag{2.1}$$

We use this formula to show

THEOREM 2.2. *For the above equally spaced points* $\|\prod_n\| \leqslant \binom{2n-1}{n}$. *Moreover, as* $m \to \infty$, $\|\prod_n\| \to \binom{2n-1}{n}$.

Proof. The trick is to consider the $l_{\mathbf{k}}$ in (2.1) as algebraic polynomials in the $m+1$ variables λ_i. Each $l_{\mathbf{k}}$ is clearly zero at the points

$$y_{\mathbf{k}} = (k_1/n, k_2/n, \ldots, k_{m+1}/n) \in \mathbb{R}^{m+1}$$

with $\sum_{i=1}^{m+1} k_i < n$, and hence so is their sum. Thus $\sum_{\mathbf{k}} l_{\mathbf{k}}$ is a polynomial of degree n in $m+1$ variables, zero at the $y_{\mathbf{k}}$ and one on the hyperplane $\sum_{i=1}^{m+1} \lambda_i = 1$ (1 is its own interpolant). But the points

$$(k_1/n, \ldots, k_{m+1}/n) \in \mathbb{R}^{m+1}, \qquad \sum_{i=1}^{m+1} k_i \leqslant n, \quad k_i \text{ nonnegative integers,}$$

are the equally spaced points of the $(m+1)$-dimensional simplex

$$\sum_{i=1}^{m+1} \lambda_i \leqslant 1, \qquad \lambda_i \geqslant 0.$$

Hence any polynomial of degree n is determined by its values at these points. Therefore

$$\sum_{\mathbf{k}} l_{\mathbf{k}} = (n^n/n!) \prod_{k=0}^{n-1} (S_1 - k/n), \qquad \text{where} \quad S_1 = \sum_{i=1}^{m+1} \lambda_i,$$

seeing that both sides agree at these points.

If we set

$$\hat{l}_{\mathbf{k}} = \left(n^n \Big/ \prod_{i=1}^{m+1} k_i!\right) \prod_{i=1}^{m+1} \prod_{k=0}^{k_i-1} (\lambda_i + k/n),$$

the same argument shows that

$$\sum_{\mathbf{k}} \hat{l}_{\mathbf{k}} = (n^n/n!) \prod_{k=0}^{n-1} (S_1 + k/n).$$

But $|l_{\mathbf{k}}| \leqslant \hat{l}_{\mathbf{k}}$ and thus $\sum_{\mathbf{k}} |l_{\mathbf{k}}| \leqslant \sum_{\mathbf{k}} \hat{l}_{\mathbf{k}} = \binom{2n-1}{n}$ on $\{S_1 = 1\} = T_m$.

To show the second statement, we actually show that

$$\lim_{m\to\infty} \sum_{\mathbf{k}} |l_{\mathbf{k}}(1/(m+1), 1/(m+1),..., 1/(m+1))|$$
$$= \lim_{m\to\infty} \sum_{\mathbf{k}} \hat{l}_{\mathbf{k}}(1/(m+1), 1/(m+1),..., 1/(m+1)) = \binom{2n-1}{n}.$$

To see this, consider a particular tuple

$$(k_1, k_2,..., k_t), \qquad k_i \geqslant 1, \quad \sum_{i=1}^{t} k_i = n, \quad t \leqslant n.$$

Exactly $\binom{m+1}{t}$ of our points have exactly t nonzero barycentric coordinates with the ith nonzero one, k_i/n above. And

$$n^{-n} \prod_{i=1}^{t} k_i! \sum_{\text{such pts.}} |l_{\mathbf{k}}(1/(m+1), 1/(m+1),..., 1/(m+1))|$$
$$= \binom{m+1}{t} \prod_{i=1}^{t} \prod_{k=0}^{k_i-1} |1/(m+1) - k/n|$$
$$= \binom{m+1}{t} (m+1)^{-t} \prod_{i=1}^{t} \prod_{k=1}^{k_i-1} |1/(m+1) - k/n| \to 1/t! \prod_{i=1}^{t} \prod_{k=0}^{k_i-1} k/n,$$

which is the same as for

$$n^{-n} \prod_{i=1}^{t} k_i! \sum_{\text{such pts.}} \hat{l}_{\mathbf{k}}(1/(m+1), 1/(m+1),..., 1/(m+1)). \qquad \blacksquare$$

3. The Points for Which |VDM| Is Greatest

In one variable, Fejér [3] showed that the points in $[-1, 1]$ which maximize $|\text{VDM}|$ are the zeros of $(1-x^2)p_n'(x)$, where p_n is the nth Legendre polynomial, and yield $\max_{[-1,1]} \sum_i l_i^2(x) = 1$. The Cauchy–Schwartz inequality gives the easy bound $\sum_i |l_i| \leqslant \sqrt{n+1}$. Sundermann [6] has shown that actually $\sum_i |l_i| = O(\log n)$ and numerical experiments conducted by Luttman and Rivlin [5] indicate that the bound of the

Lebesgue function corresponding to these points is slightly smaller than that corresponding to the near-optimal Chebyshev points.

Unfortunately, for $m > 1$ things are somewhat more complicated. We do have

THEOREM 3.1. *If $x_i \in T_m$, $1 \leqslant i \leqslant N$ are such that* $\max_{x \in T_m} \sum_i l_i^2(x) = 1$, *then these points also maximize* $|\mathrm{VDM}|$.

Proof. Any monomial $m_j(x) \in \mathbb{P}_n^m$ is its own interpolant. Hence

$$m_j(x) = \sum_{i=1}^{N} m_j(x_i)\, l_i(x), \qquad 1 \leqslant j \leqslant N.$$

In particular, if y_k, $1 \leqslant k \leqslant N$, is any other configuration of points in T_m,

$$m_j(y_k) = \sum_{i=1}^{N} m_j(x_i)\, l_i(y_k), \qquad 1 \leqslant j, \quad k \leqslant N.$$

This equation may be regarded as matrix multiplication.

$$\begin{pmatrix} m_1(y_1) & m_2(y_1) \cdots m_N(y_1) \\ m_1(y_2) & m_2(y_2) \cdots m_N(y_2) \\ \vdots & \vdots \\ m_1(y_N) & m_2(y_N) \cdots m_N(y_N) \end{pmatrix}$$
$$= \begin{pmatrix} l_1(y_1) & l_2(y_1) \cdots l_N(y_1) \\ l_1(y_2) & l_2(y_2) \cdots l_N(y_2) \\ \vdots & \vdots \\ l_1(y_N) & l_2(y_N) \cdots l_N(y_N) \end{pmatrix} \begin{pmatrix} m_1(x_1) \cdots m_N(x_1) \\ m_1(x_2) \cdots m_N(x_2) \\ \vdots \quad \vdots \\ m_1(x_N) \cdots m_N(x_N) \end{pmatrix}. \tag{3.2}$$

Now each row of the matrix below has, by assumption, l_2 length at most one. By Hadamard's inequality, therefore,

$$\left| \det \begin{pmatrix} l_1(y_1) & l_2(y_1) \cdots l_N(y_1) \\ l_1(y_2) & l_2(y_2) \cdots l_N(y_2) \\ \vdots & \vdots \\ l_1(y_N) & l_2(y_N) \cdots l_N(y_N) \end{pmatrix} \right| \leqslant 1.$$

Thus, taking determinants of (3.2), we have

$$|\mathrm{VDM}(y_1, y_2, \ldots, y_N)| \leqslant |\mathrm{VDM}(x_1, x_2, \ldots, x_N)|. \qquad \blacksquare$$

However, the converse is apparently not true. Numerical work with the $m=2$, $n=5$ case suggests

Conjecture 3.3. The converse to Theorem 3.1 is not necessarily true. Moreover, $\max_{x\in T_m}\sum_i l_i^2(x)=1$ is not always attainable. ▮

For the case of X a square in $\mathbb{R}^2$, the example of $n=1$ shows this conjecture to be true for a general region.

EXAMPLE 3.4. Let $X=\{(x,y): 0\leqslant x, y\leqslant 1\}$. For degree $n=1$, $N=3$ and

$$\mathrm{VDM}(x_1,x_2,x_3)=\begin{vmatrix} 1 & u_1 & v_1 \\ 1 & u_2 & v_2 \\ 1 & u_3 & v_3 \end{vmatrix},$$

where $x_i=(u_i,v_i)$. Since VDM is twice the (signed) area of the triangle with vertices at the x_i, its modulus is clearly maximized by having two points at two vertices of X and the third *anywhere* on the opposite side. For the specific case of the x_i being $(0,0)$, $(1,0)$, and $(h,1)$, it is easily seen that

$$l_1(u,v)=v(h-1)+1-u, \qquad l_2(u,v)=u-hv, \qquad l_3(u,v)=v.$$

Hence $\sum_{i=1}^3 l_i^2(u,v)=2(h^2-h+1)v^2+2u^2+2(1-2h)uv+2(h-1)v-2u+1$, which is $2h^2+1$ at $(0,1)$ and $2(h-1)^2+1$ at $(1,1)$. Therefore $\min_{0<h<1}\max_{(u,v)\in X}\sum_i l_i^2(u,v)>1$. ▮

However, the points which maximize $|\mathrm{VDM}|$ do allow the immediate bound $\max_{x\in T_m}\sum_{i=1}^N |l_i(x)|\leqslant N$. This follows directly from the fact that

$$l_i(x)=\frac{\mathrm{VDM}(x_1,x_2,\ldots,x_{i-1},x,x_{i+1},\ldots,x_N)}{\mathrm{VDM}(x_1,x_2,\ldots,x_N)}$$

and hence, for these points, $\max_{x\in T_m}|l_i(x)|=1$.

This bound, as will become clear, is extremely pessimistic.

Now, the function $\mathrm{VDM}(x_1,x_2,\ldots,x_N)$ can easily be maximized numerically, but in order to get analytic expressions for the points, at least for low degrees, we look at the configuration of the equally spaced points and hope that the configuration of these maximum points is qualitatively similar.

LEMMA 3.5. *The* $\binom{n+m}{m}$ *equally spaced points of degree* n *lie on* $\lfloor (n-1)/(m+1)\rfloor+1$ *concentric simplexes in such a manner that* $\binom{n-i(m+1)+m}{m}-\binom{n-(i+1)(m+1)+m}{m}$ *of them lie on the ith simplex* (*proceeding from the outside*), $0\leqslant i\leqslant\lfloor (n-1)/(m+1)\rfloor$. *They have the further property* *that exactly* $\binom{n-1}{q}$ *points lie in the* interior *of each q-face of* T_m, $0 \leqslant q \leqslant m-1$.

Proof. The first statement follows easily from the fact that the number of points *interior* to T_m is $\binom{n-(m+1)+m}{m}$ (we take $\binom{k}{m}=0$ if $k<m$). To see this, note that the interior points are those whose barycentric coordinates are of the form $(k_1/n, k_2/n,..., k_{m+1}/n)$, $1 \leqslant k_i$. By subtracting 1 from each of the $m+1$ k_i, we see that the number of such points is the same as the number of equally spaced points of degree $n-(m+1)$, $\binom{n-(m+1)+m}{m}$.

To see the second statement, note that the points *interior* to a particular q-face are those for which a fixed $m+1-(q+1)$ of the λ_i are zero and the $q+1$ remaining coordinates are nonzero. The number of such of the equally spaced points is clearly, then, the same as the number of tuples

$$(k_1/n, k_2/n,..., k_{q+1}/n), \qquad k_i > 0 \quad \text{and} \quad \sum_{i=1}^{q+1} k_i = n.$$

By the previous argument, this number is $\binom{n-(q+1)+q}{q} = \binom{n-1}{q}$. ∎

We propose to take points in this same type of configuration and adjust the "radii" of the concentric simplexes and how the points lie on each face, so as to maximize $|\mathrm{VDM}|$, if possible.

One immediate advantage of placing the points in this configuration is that then the Lagrange polynomials can be calculated in a simple inductive manner. This is best seen through an example.

EXAMPLE 3.6. Take $n=4$, $N=15$, and X a triangle in $\mathbb{R}^2$. The scheme tells us to put 1 point at each vertex, $\binom{4-1}{3}=3$ in the interior of each face and the remaining three at the vertices of a concentric triangle as in Fig. 1.

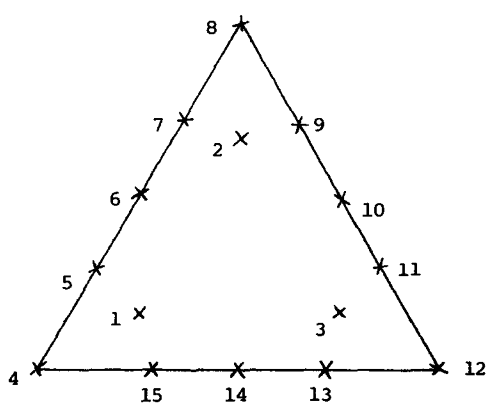

FIGURE 1

Here l_1 is simply the product of the three face equations together with the equation of the line going through x_2 and x_3, normalized to be 1 at x_1.

For a point such as x_5, we use the one-dimensional theory to find a polynomial, p, say, of degree 2 such that $p(x_5)=1$ but $p(x_6)=p(x_7)=0$. Multiplying p by the equations of the other two faces gives us a polynomial q of degree 4 which when normalized has the desired values of l_5 on the boundary of the triangle. To get l_5, we need only subtract the right values from q so that $l_5(x_1)=l_5(x_2)=l_5(x_3)=0$. That is, $l_5(x)=q(x)-\sum_{i=1}^{3} q(x_i)\, l_i(x)$.

To find the Lagrange polynomial for x_8, a vertex, let $p(x)$ be chosen so that $p(x)=0$ is the face opposite to x_8. Then clearly $l_8(x)=p(x)-\sum_{i=1, i\neq 8}^{11} p(x_i)\, l_i(x)$ suitably normalized. ∎

We proceed now to calculate VDM for the $\mathbb{R}^2$ case. It is convenient to take a standardized triangle: that with vertices at $(0, 1)$ and $(\pm\sqrt{3}/2, -1/2)$. The equations of the three faces are $y+\sqrt{3}x-1=0$, $y-\sqrt{3}x-1=0$ and $y+1/2=0$. Denote by Δ_R the concentric triangle of radius R, i.e., that whose face equations are $y+\sqrt{3}x-R=0$, $y-\sqrt{3}x-R=0$, and $y+R/2=0$. Our scheme is to place $\binom{n-3i+2}{2}-\binom{n-3i-1}{2}=3(n-3i)$ points on the ith triangle Δ_{R_i}, $0\leqslant i\leqslant \lfloor (n-1)/3\rfloor = s$. We place the points on the faces of Δ_{R_i} so as to maximize the one-dimensional VDM of degree $n-3i$ as per Fejér's theorem. Note that if $3\mid n$, one point will lie at the centre of the triangle.

Proposition 3.7. *For the above described points* VDM *is a nonzero multiple of*

$$\prod_{i=0}^{s}\left(R_i^{t_i}\prod_{k=i+1}^{s} R_k^{6(n-3k)}(R_k-R_i)^{3(n-3k)}(p'_{n-3k}((R_k+2R_i)/(3R_k)))^6\right.$$
$$\left.\times\,(((R_k+2R_i)/(3R_k))^2-1)^3\right),$$

where

$$\begin{aligned} t_i &= 2\binom{n-3i+2}{3}-2\binom{n-3i-1}{3}-9\sum_{k=i+1}^{s}(n-3k)\\ &=(3/2)\,n(n+1)-9ni+(27i^2-9i+4)/2, \qquad \textit{if}\;\; 3\mid n,\\ &=(3/2)\,n(n+1)-9ni+(27i^2-9i-2)/2 \qquad \textit{otherwise,}\end{aligned}$$

and p_k is the kth Legendre polynomial.

Proof. The proof is long and computational but not difficult. Basically, we row reduce the determinant using the relationships generated by the fact that groups of points are colinear. It is not included here. ∎

This polynomial in the radii can be maximized analytically for degree up to 4 and numerically for higher degrees to generate reasonably good interpolation points. A partial table of numerical bounds on the Lebesgue function follows.

Degree	No. Pts.	Radii	$\max \sum \lvert l_i \rvert$	
1	3	1	1	1
2	6	1	$1\frac{2}{3}$	$1\frac{2}{3}$
3	10	1, 0	2.105	2.26
4	15	$1, (1+3\sqrt{5})/22$	2.726	3.47
5	21	1, 0.546713389	3.8665	5.23
6	28	1, 0.662591473, 0	4.5111	8.48
7	36	1, 0.7392097205, 0.2099178923	5.5187	14.33

The rightmost column is the numerical bound on the Lebesgue function for the corresponding equally spaced points.

For low degrees, these radii also determine the points for higher dimensional simplexes T_m.

For degree 1, the scheme tells us to put 1 point at each of the $m+1$ vertices v_i. These are the equally spaced points of degree 1. We know that, in barycentric coordinates, $l_i = \lambda_i$ and hence $\sum_{i=1}^{m+1} l_i^2 = \sum_{i=1}^{m+1} \lambda_i^2 \leqslant 1$ on T_m. By Theorem 3.1 these points also maximize $|\mathrm{VDM}|$. Moreover, $\sum_i |l_i| = \sum_i l_i = 1$.

For degree 2, we put 1 point at each of the $m+1$ vertices v_i and 1 point at each of the $\binom{m+1}{2}$ midpoints, $(v_i + v_j)/2$, $i \neq j$. These are the equally spaced points of degree 2. Hence, the Lagrange polynomial corresponding to a vertex v_i is $l_i = 2\lambda_i(\lambda_i - \frac{1}{2})$ and that to $(v_i + v_j)/2$ is $l_{ij} = 4\lambda_i\lambda_j$. These points also maximize $|\mathrm{VDM}|$, as follows from

Proposition 3.8. *For the above points,* $\sum_i l_i^2 \leqslant 1$ *on* T_m.

Proof. We proceed by induction. The case $m = 1$ is handled by Fejér's theorem. Now suppose the proposition to be true for dimensions $<m$. Then $p = \sum_i l_i^2 \leqslant 1$ on the skin of the simplex T_m, and so if $\max p > 1$, its maximum can only be attained in the interior. Supposing this to be the case, let x^* be a max point of p. By direct computation, $p(1/(m+1), 1/(m+1), \ldots, 1/(m+1)) = (m^2 + 6m + 1)/(m+1)^3 < 1$ for $m > 1$ and so x^* is not the centre of T_m. By symmetry, then, there exists a $y^* \neq x^*$ also a max point of p.

Now consider p restricted to the line going through x^* and y^*. It is a strictly positive quartic with *two* local max points and so must be a constant. But this possibility is eliminated by Lemma 3.9 below. Thus the assumption that $p > 1$ somewhere on T_m must be false. ∎

LEMMA 3.9. *Suppose that* $x_i \in \mathbb{R}^m$, $1 \leqslant i \leqslant N_n^m$ *are such that* $\mathrm{VDM}(x_1, \ldots, x_N) \neq 0$. *Then for any* $c \geqslant 0$, $V = \{x \in \mathbb{R}^m : \sum_{i=1}^N l_i^2 = c\}$ *is bounded.*

Proof. Let $\pi_k(x)$ be the kth coordinate function. Then $\pi_k(x) = \sum_{i=1}^N \pi_k(x_i)\, l_i(x)$ and by Cauchy–Schwartz $|\pi_k(x)|^2 \leqslant (\sum_{i=1}^N \pi_k^2(x_i))(\sum_{i=1}^N l_i^2(x))$. Thus for $x \in V$, $|\pi_k(x)|^2 \leqslant c \sum_{i=1}^N \pi_k^2(x_i)$ and the result follows. ∎

Now we know from Theorem 2.2 that the Lebesgue function for these points is bounded by 3. A slightly better bound is available.

PROPOSITION 3.10. *For the above points,* $\sum_i |l_i| \leqslant \sum_i |l_i(1/(m+1), \ldots, 1/(m+1))| = (3m-1)/(m+1)$ *if* $m > 1$.

Proof. The Lagrange polynomials of the form $4\lambda_i\lambda_j$ are nonnegative on T_m. We need only consider the sign changes of those of the form $2\lambda_i(\lambda_i - 1/2)$. Now since $\sum_i \lambda_i = 1$ and $\lambda_i \geqslant 0$, it is clear that the possible sign patterns are

(i) $2\lambda_k(\lambda_k - 1/2) \geqslant 0$ and $2\lambda_j(\lambda_j - 1/2) \leqslant 0$ for all $j \neq k$;

(ii) $2\lambda_i(\lambda_i - 1/2) \leqslant 0$ $1 \leqslant i \leqslant m+1$.

Consider first case (ii). This being the case

$$\sum_i |l_i| = \sum_{i<j} 4\lambda_i\lambda_j - \sum_i 2\lambda_i(\lambda_i - \tfrac{1}{2}).$$

But $1 = \sum_i l_i = \sum_{i<j} 4\lambda_i\lambda_j + \sum_i 2\lambda_i(\lambda_i - \frac{1}{2})$ and so $\sum_{i<j} 4\lambda_i\lambda_j = 1 - \sum_i 2\lambda_i(\lambda_i - \frac{1}{2})$. Hence

$$\begin{aligned}\sum_i |l_i| &= 1 - 4\sum_i \lambda_i(\lambda_i - \tfrac{1}{2}) = 1 - 4\sum_i \lambda_i^2 + 2\sum_i \lambda_i \\ &= 3 - 4\sum_i \lambda_i^2 \leqslant 3 - 4/(m+1) = (3m-1)/(m+1).\end{aligned}$$

For case (i), suppose that it is $2\lambda_k(\lambda_k - \frac{1}{2}) \geqslant 0$ and $2\lambda_j(\lambda_j - \frac{1}{2}) \leqslant 0, j \neq k$. Then

$$\begin{aligned}\sum_i |l_i| &= \sum_{i<j} 4\lambda_i\lambda_j - \sum_{j \neq k} 2\lambda_j(\lambda_j - \tfrac{1}{2}) + 2\lambda_k(\lambda_k - \tfrac{1}{2}) \\ &= \sum_{i<j} 4\lambda_i\lambda_j - \sum_j 2\lambda_j(\lambda_j - \tfrac{1}{2}) + 4\lambda_k(\lambda_k - \tfrac{1}{2}) \\ &= 1 - 4\sum_j \lambda_j(\lambda_j - \tfrac{1}{2}) + 4\lambda_k(\lambda_k - \tfrac{1}{2}) \\ &= 3 - 4\sum_{j \neq k} \lambda_j^2 - 2\lambda_k.\end{aligned}$$

Elementary considerations show that this last expression is bounded by $(3m-1)/(m+1)$. ∎

For degree 3, the scheme tells us to put the points at

$$(v_i + v_j + v_k)/3, \qquad i < j < k, \quad \text{(centre of each 2-dimensional face)},$$
$$v_i(1 + 1/\sqrt{5})/2 + v_j(1 - 1/\sqrt{5})/2, \qquad i \neq j \quad \text{(interior of each 1-face)},$$

and

$$v_i, \qquad 1 \leqslant i \leqslant m+1 \quad \text{(each vertex)}.$$

The Lagrange polynomials can be computed as in Example 3.6 to be

$$l_{ijk} = 27\lambda_i\lambda_j\lambda_k,$$
$$l_{ij} = 5\lambda_i\lambda_j(\lambda_i(3+\sqrt{5})/2 + \lambda_j(3-\sqrt{5})/2 - 1),$$

and

$$l_i = (\lambda_i/2)(12\lambda_i^2 - 12\lambda_i + 3 - S_2),$$

respectively, where we write $S_k = \sum_{i=1}^{m+1} \lambda_i^k$.

We conjecture that these points do indeed maximize $|\text{VDM}|$ but can only prove so for $m \leqslant 2$. For $m = 2$, it suffices to take X to be the standardized triangle of Proposition 3.7. In this case these ten points are

$$(0, 1), \quad (\pm\sqrt{3}/2, -1/2), \quad (\pm\sqrt{3}/(2\sqrt{5}), -1/2),$$
$$(\pm\sqrt{3}/4(1 \pm 1/\sqrt{5}), \quad 1 - 3/4(1 \pm 1/\sqrt{5})), \quad (0, 0).$$

PROPOSITION 3.11. *For degree* 3, $m = 2$, *the above* 10 *points yield* $\max_{x \in X} \sum_i l_i^2(x) = 1$.

Proof. Since we have formulas for the l_i, we can also compute $\sum_i l_i^2$, which after laborious calculations is seen to be, in Cartesian coordinates,

$$1 - (262/81)y^2 + (424/81)y^3 + (154/27)y^4 - (1796/81)y^5 + (1172/81)y^6$$
$$- (262/81)x^2 - (424/27)x^2y + (308/27)x^2y^2 + (3592/81)x^2y^3$$
$$+ (356/27)x^2y^4 + (154/27)x^4 + (1796/27)x^4y + (572/9)x^4y^2 + (100/9)x^6$$

or, in polar coordinates,

$$\begin{aligned}
&1 - (262/81)r^2 + (154/27)r^4 + (1036/81)r^6 \\
&+ ((1796/81)r^2 - 424/81)r^3 \operatorname{Sin} 3\theta - (136/81)r^6 \operatorname{Cos} 6\theta \\
&\qquad = 1 - (262/81)r^2 + (154/27)r^4 + (1036/81)r^6 \\
&\qquad\quad + ((1796/81)r^2 - 424/81)r^3u \\
&\qquad\quad - (136/81)r^6(1 - 2u^2), \qquad \text{where} \quad u = \operatorname{Sin} 3\theta.
\end{aligned}$$

Since the coefficient of u^2 is $(272/81)\,r^6 > 0$ if r is, the critical point of the above polynomial, considered as a quadratic in u, is a minimum point and hence the maximum must be attained only at the boundary values $u = \pm 1$. But $\operatorname{Sin} 3\theta = \pm 1$ at $\theta = (2k+1)\pi/6$, $0 \leqslant k \leqslant 5$ which corresponds to three lines through the origin, one of which is $x = 0$.

Now $\sum_i l_i^2 \leqslant 1$ on the boundary of the triangle because of the one-dimensional case and so $\sum_i l_i^2 \leqslant 1$ on these three line segments is sufficient for this being true throughout the triangle. By symmetry, the line segment $x = 0$, $-1/2 \leqslant y \leqslant 1$ suffices. But on $x = 0$,

$$\begin{aligned} p(y) = \sum_i l_i^2(0, y) &= 1 - (262/81)\,y^2 + (424/81)\,y^3 + (154/27)\,y^4 \\ &\quad - (1796/81)\,y^5 + (1172/81)\,y^6 \\ &= 1 + (2/81)\,y^2(y-1)(586y^3 - 312y^2 - 81y + 131). \end{aligned}$$

By elementary means, $586y^3 - 312y^2 - 81y + 131 \geqslant 0$ on $[-1/2, 1]$ and thus $p(y) \leqslant 1$ on $[-1/2, 1]$. ∎

We can, however, bound the Lebesgue function for arbitrary dimensions.

PROPOSITION 3.12. *For the above points* $\sum_i |l_i| \leqslant 11 - 9/(m+1)$.

Proof. For the vertices,

$$\begin{aligned} |l_i| &\leqslant |\lambda_i/2\{12\lambda_i^2 - 12\lambda_i + 3 - S_2\}| \\ &= |\lambda_i/2\{12(\lambda_i - 1/2)^2 - S_2\}| \\ &\leqslant \lambda_i/2\{12(\lambda_i - 1/2)^2 + S_2\}. \end{aligned}$$

Hence

$$\begin{aligned} \sum_{i=1}^{m+1} |l_i| &\leqslant \sum_{i=1}^{m+1} \lambda_i/2\{12(\lambda_i - 1/2)^2 + S_2\} \\ &= \tfrac{1}{2}\{12S_3 - 12S_2 + 3 + S_2\} = \tfrac{1}{2}\{3 - 11S_2 + 12S_3\}. \end{aligned}$$

For the points on the one-dimensional faces,

$$\begin{aligned} |l_{ij}| &= |5\lambda_i\lambda_j\{\lambda_i(3+\sqrt{5})/2 + \lambda_j(3-\sqrt{5})/2 - 1\}| \\ &\leqslant 5\lambda_i\lambda_j\{\lambda_i(3+\sqrt{5})/2 + \lambda_j(3-\sqrt{5})/2 - 1\}. \end{aligned}$$

Hence

$$\begin{aligned} \sum_{i<j} |l_{ij}| + |l_{ji}| &\leqslant \sum_{i<j} 5\lambda_i\lambda_j\{3(\lambda_i + \lambda_j) + 2\} = 5\left\{3\sum_{i\neq j} \lambda_i^2\lambda_j + \sum_{i\neq j} \lambda_i\lambda_j\right\} \\ &= 5\{3(S_2 - S_3) + (1 - S_2)\} = 5\{1 + 2S_2 - 3S_3\}. \end{aligned}$$

For the points at the centres of the two-dimensional faces,

$$|l_{ijk}| = |27\lambda_i\lambda_j\lambda_k| = 27\lambda_i\lambda_j\lambda_k.$$

Hence

$$\sum_{i<j<k} |l_{ijk}| = (27/3!) \sum_{\substack{i,j,k \\ \text{distinct}}} \lambda_i\lambda_j\lambda_k$$
$$= (9/2)\{1 - 3S_2 + 2S_3\}.$$

Adding the three estimates, we see that

$$\sum_{i=1}^{N} |l_i| \leqslant \tfrac{1}{2}(3 - 11S_2 + 12S_3) + 5(1 + 2S_2 - 3S_3) + \tfrac{9}{2}(1 - 3S_2 + 2S_3)$$
$$= 11 - 9S_2$$
$$\leqslant 11 - 9/(m+1). \quad \blacksquare$$

For $m \geqslant 3$ we conjecture that actually the maximum of the Lebesgue function is its value at the centre of the simplex. This value is easily computed to be $(11m^2 - 18m + 1)/(m+1)^2$.

This last calculation shows that the bound of Proposition 3.12 is *asymptotically* sharp. On the negative side, it also shows that the Lebesgue function for these points is asymptotically larger than that of the equally spaced points, which, by Theorem 2.2, is bounded by 10.

For degree 4, the scheme tells us to place the points at

$$(v_i + v_j + v_k + v_l)/4, \qquad i<j<k<l$$
(centre of each 3-face); (3.13.1)

$$v_i(4+\sqrt{5})/11 + (v_j + v_k)(7-\sqrt{5})/22, \qquad i \neq j, k, \quad j<k$$
(concentric triangle in each 2-face of relative radius $(1 + 3\sqrt{5})/22$); (3.13.2)

$$v_i(1-\sqrt{3/7})/2 + v_j(1+\sqrt{3/7})/2, \qquad i \neq j$$
(3 pts. in the interior of each 1-face); (3.13.3)

$$(v_i + v_j)/2, \qquad i<j; \qquad (3.13.4)$$

$$v_i, \qquad 1 \leqslant i \leqslant m+1. \qquad (3.13.5)$$

The Lagrange polynomials can again be computed as in Example 3.6 to be

$$
\begin{aligned}
l_{ijkl} &= 256\lambda_i\lambda_j\lambda_k\lambda_l,\\
l_{ijk} &= (73+\sqrt{5})/2\lambda_i\lambda_j\lambda_k\{(1+\sqrt{5})\,\lambda_i + (\lambda_j+\lambda_k)(3-\sqrt{5})/2-1\}\\
l_{ij} &= 49/6\lambda_i\lambda_j\{((61+7\sqrt{5})/22-\sqrt{3/7}(7+\sqrt{5})/2)\,\lambda_i^2\\
&\quad +\lambda_i\lambda_j(3+9\sqrt{5})/11+((61+7\sqrt{5})/22+\sqrt{3/7}(7+\sqrt{5})/2)\,\lambda_j^2\\
&\quad +(\sqrt{3/7}(5+\sqrt{5})/2-(41+13\sqrt{5})/22)\,\lambda_i\\
&\quad -(\sqrt{3/7}(5+\sqrt{5})/2+(41+13\sqrt{5})/22)\,\lambda_j\\
&\quad +2(4+\sqrt{5})/11+S_2(\sqrt{5}-7)/11\},\\
l_{ij} &= 4/33\lambda_i\lambda_j\{(100-8\sqrt{5})(\lambda_i^2+\lambda_j^2)+(672-96\sqrt{5})\,\lambda_i\lambda_j\\
&\quad +(62\sqrt{5}-302)(\lambda_i+\lambda_j)+(76-14\sqrt{5})+(82-40\sqrt{5})\,S_2\},\\
l_i &= 2\lambda_i\{\lambda_i^3(101+17\sqrt{5})/11-(13+2\sqrt{5})\,\lambda_i^2+\lambda_i(130+27\sqrt{5})/22\\
&\quad -(259+51\sqrt{5})/264+S_2((9+\sqrt{5})/8-\lambda_i(24+17\sqrt{5/22}))\\
&\quad +S_3((45+3\sqrt{5})/44-5/3)\},
\end{aligned}
$$

respectively.

We conjecture that these points do maximize $|\mathrm{VDM}|$, but again can only prove so for dimensions up to two. Taking X to be the standardized triangle as before, we have

Proposition 3.14. *For degree* 4 *and* $m=2$, *the above* 15 *points yield* $\max_{x\in X}\sum_i l_i^2(x)=1$.

Proof. Again by direct calculation we find that, in polar coordinates,

$$
\begin{aligned}
\sum_{i=1}^{15} l_i^2 &= (48109+2416\sqrt{5})/72171+(66541-11327\sqrt{5})/6561r^2\\
&\quad +(177068\sqrt{5}-135340)/72171r^3\,\mathrm{Sin}\,3\theta\\
&\quad +(245081\sqrt{5}-1724917)/24057r^4\\
&\quad -(238490\sqrt{5}+3893138)/72171r^5\,\mathrm{Sin}\,3\theta\\
&\quad +(82072-11612\sqrt{5})/729r^6\\
&\quad +(487384-29816\sqrt{5})/2187r^7\,\mathrm{Sin}\,3\theta\\
&\quad +(308800-13184\sqrt{5})/6561r^8\,\mathrm{Sin}^2\,3\theta\\
&\quad +(1507408-363800\sqrt{5})/72171r^6\,\mathrm{Sin}^2\,3\theta+3290/81r^8.
\end{aligned}
$$

Since both $(308800-13184\sqrt{5})/6561$ and $(1507408-363800\sqrt{5})/72171$ are positive, this function is a quadratic in $\mathrm{Sin}\,3\theta$ with positive leading coefficient. Hence, as before, it suffices to show that $\sum_i l_i^2 \leqslant 1$ on the segment $x=0$ and $-\frac{1}{2} \leqslant y \leqslant 1$. But on $x=0$, $p(y)=\sum_{i=1}^{15} l_i^2(0,y)$ is such that

$$\begin{aligned}
&72171(p(y)-1)\\
&\quad = 22(y-1)(y+1/2)(y-(1+3\sqrt{5})/22)^2\{(313160-6592\sqrt{5})\,y^4\\
&\qquad + (-555016+126236\sqrt{5})\,y^3 + (399504-194520\sqrt{5})\,y^2\\
&\qquad + (-140711+92023\sqrt{5})\,y + (26803-5807\sqrt{5})\}.
\end{aligned}$$

Therefore $p(y) \leqslant 1$ on $[-1/2, 1]$ is equivalent to the quartic in brace brackets being positive on this interval, which is verified by laborious but elementary means. ∎

We can again bound the Lebesgue function for these points for arbitrary dimensions.

PROPOSITION 3.15. *For the above points the Lebesgue function is bounded by* $(1367+42\sqrt{5})/33-(289-127\sqrt{5})/(6(m+1))-(622\sqrt{5}-614)/(33(m+1)^2)$.

Proof. The idea of the proof is the same as for the degree 3 case: we bound the sum of the absolute values of the Lagrange polynomials grouped according to the "type" of point to which they correspond. The computations are not particularly pleasant.

For the points of (3.13.1),

$$\begin{aligned}
\sum |l_{ijkl}| &= (256/4!) \sum_{\substack{i,j,k,l\\ \text{distinct}}} \lambda_i\lambda_j\lambda_k\lambda_l\\
&= (32/3)(1-6S_2+3S_2^2+8S_3-6S_4).
\end{aligned}$$

For the points of (3.13.2)

$$\begin{aligned}
|l_{ijk}| &= |(73+\sqrt{5})/2\lambda_i\lambda_j\lambda_k\{(1+\sqrt{5})\,\lambda_i+(\lambda_k+\lambda_j)(3-\sqrt{5})/2-1\}|\\
&\leqslant (73+\sqrt{5})/2\lambda_i\lambda_j\lambda_k\{(1+\sqrt{5})\,\lambda_i+(\lambda_k+\lambda_j)(3-\sqrt{5})/2+1\}.
\end{aligned}$$

Hence $|l_{ijk}|+|l_{kij}|+|l_{jki}| \leqslant (73+\sqrt{5})/2\lambda_i\lambda_j\lambda_k\{4(\lambda_i+\lambda_j+\lambda_k)+3\}$ and

$$\begin{aligned}
&\sum |l_{ijk}|+|l_{kji}|+|l_{jki}|\\
&\qquad \leqslant (73+\sqrt{5})/(2\ 3!) \sum_{\substack{i,j,k\\ \text{distinct}}} \lambda_i\lambda_j\lambda_k\{4(\lambda_i+\lambda_j+\lambda_k)+3\}\\
&\qquad = (73+\sqrt{5})/4(1+S_2-4S_2^2-6S_3+8S_4).
\end{aligned}$$

For the points (3.13.3), we can by similar techniques show that

$$\sum |l_{ij}| + |l_{ji}| \leqslant (49/33)(4 + \sqrt{5} + (20 + 5\sqrt{5})\, S_2 + (5\sqrt{5} - 2)\, S_2^2 + (10 - 3\sqrt{5})\, S_3 - (32 + 8\sqrt{5})\, S_4).$$

For the points (3.13.4) we can show that

$$\sum |l_{ij}| \leqslant (4/33)(38 - 7\sqrt{5} + (89\sqrt{5} - 381)\, S_2 + (377 - 68\sqrt{5})\, S_2^2 + (402 - 70\sqrt{5})\, S_3 + (56\sqrt{5} - 436)\, S_4).$$

Lastly, for the points (3.13.5) we show that

$$\sum |l_i| \leqslant (259 + 51\sqrt{5})/132 + ((9 + \sqrt{5})/4 + (130 + 27\sqrt{5})/11)\, S_2 + (24 + 17\sqrt{5})/11 S_2^2 - (68/3 + (45 + 91\sqrt{5})/22)\, S_3 + 2(101 + 17\sqrt{5})/11 S_4.$$

Adding up the five estimates, we see that

$$\begin{aligned}\sum_{i=1}^{N} |l_i| &\leqslant (1367 + 42\sqrt{5})/33 + ((127\sqrt{5} - 289)/6)\, S_2 \\ &\quad + ((43 - 3\sqrt{5})/11)\, S_2^2 \\ &\quad + ((485 - 613\sqrt{5})/33)\, S_3 \\ &\leqslant (1367 + 42\sqrt{5})/33 + ((127 - 289\sqrt{5})/6)\, S_2 \\ &\quad + ((614 - 622\sqrt{5})/33)\, S_3,\end{aligned}$$

where we have used the fact that $S_2^2 \leqslant S_3$. The result follows from $S_2 \geqslant 1/(m+1)$ and $S_3 \geqslant 1/(m+1)^2$. ∎

Seeing that for dimensions at least 4, all the points lie on the boundary of T_m, a reasonable conjecture is that for $m \geqslant 4$ the maximum of the Lebesgue function is its value at the centre of the simplex. This value is easily computed to be $((1367 + 42\sqrt{5})\, m^3 - (5259 + 168\sqrt{5})\, m^2 + (4189 + 126\sqrt{5})\, m - 33)/(33(m+1)^3)$. The bound of Proposition 3.15 is thus asymptotically best possible.

Unfortunately, for degrees higher than 5 this scheme does not produce the points which maximize $|\mathrm{VDM}|$.

EXAMPLE 3.16. For $n = 5$, $N = 21$ in $\mathbb{R}^2$, the scheme tells us to place 15 points on the boundary of the triangle and six on a concentric triangle whose radius is determined by maximizing the polynomial of Proposition 3.7, which in this case is $R^8(R-1)^9(R+2)^6(2R+1)^3$. Taking the derivative, we see that this value of R is a root of $52R^3 + 69R^2 - 24R - 16 = 0$. But the Lagrange polynomial corresponding to $(0, R)$ is easily seen to be

$$l(x, y) = c(y - \sqrt{3}x - 1)(y + \sqrt{3}x - 1)(y + 1/2)(y + R/2)(y - R/4)$$

for a suitable constant c. Thus $(\partial l/\partial y)(0, R) = 0$ iff $5R^2 - R - 1 = 0$.

But $5R^2 - R - 1$ and $52R^3 + 69R^2 - 24R - 16$ have no common root and so $(0, R)$ cannot be a max point of $l(x, y)$. Hence there exists an (x, y) in X for which $|l(x, y)| > 1$ and these points cannot maximize $|\text{VDM}|$. ∎

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